

PROSIMPLUS APPLICATION EXAMPLE

PRICO PROCESS: NATURAL GAS LIQUEFACTION

	EXAMPLE PURPOSE				
	This example presents the simulation of the PRICO process for the liquefaction of natural gas with a refrigeration cycle. This process is analyzed with the pinch and exergy analysis.				
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1. Process modeling

1.1. Process description

This example presents a liquefaction plant for natural gas. This process requires a large amount of energy because the gas has to be cooled down to a temperature of about -160°C. The PRICO process is one of the simplest processes for the liquefaction of natural gas. It is made of only one cycle. This example is inspired by the case study presented in the PhD thesis of D. Marmolejo Correa (2013) [MAR21].

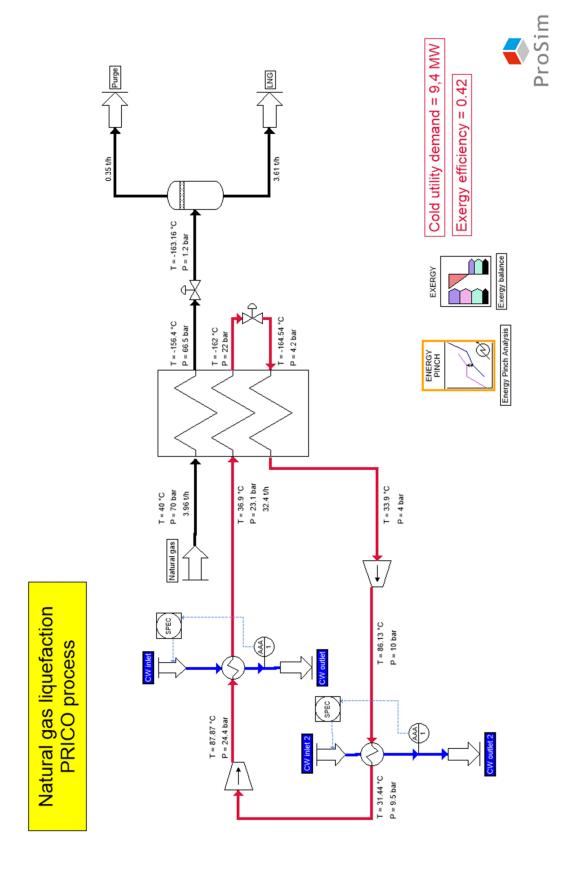
The PRICO process operates with a mixture of refrigerants made of nitrogen, methane, ethane, propane, n-butane and isopentane. The refrigerant is compressed, then partially condensed before entering in the cold chamber where it is fully condensed at -162°C. The fluid is then expanded and heated in the same multi-fluid heat exchanger. The amount of heat extracted from heating the refrigerant is used to liquefy the natural gas around -160°C. At this temperature, the less volatile hydrocarbons are condensed. The mixture then enters in a flash column where the heaviest hydrocarbons are extracted in liquid state. The liquid output is the LNG (Liquefied Natural Gas). The uncondensed gas is returned to the cold chamber for recycling (this last part is not simulated in this case study) [STE75].

This mature process has been used in China for the peak-shaving of LNG stations and for gas stations with the goal of substituting fuels, gasoline and diesel, with liquefied natural gas (LNG).

Pinch analysis and exergy analysis are presented to study the PRICO process.

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1.2. Simulation flowsheet



Simulation of a natural gas liquefaction process

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1.3. Components

The components taken into account in the simulation are listed in the table below, as well as their chemical formula and their CAS numbers¹. The properties of pure substances are taken from the standard ProSim database [WIL21].

Component	Chemical formula	CAS Number (1)
Nitrogen	N_2	7727-37-9
Methane	CH ₄	74-82-8
Ethane	C_2H_6	74-84-0
Propane	C_3H_8	74-98-6
n-Butane	C_4H_{10}	106-97-8
Isobutane	C_4H_{10}	75-28-5
Isopentane	C_5H_{12}	78-78-4
Water	H ₂ O	7732-18-5

¹ CAS Registry Numbers® are the intellectual property of the American Chemical Society and are used by ProSim SA with the express permission of ACS. CAS Registry Numbers® have not been verified by ACS and may be inaccurate.

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1.4. Thermodynamic model

Two thermodynamic "calculators" are defined in this simulation:

- ➤ "PSRK": this calculator is used for the global flowsheet, except for cooling streams of pure water. The thermodynamic profile used is PSRK.
- > "Water": this calculator is used for cooling streams of pure water. The thermodynamic model is the specific pure water model.

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1.5. **Operating conditions**

√ Feeds

Name:	CW inlet	CW inlet 2	Natural gas
	Mass fractions	Mass fractions	Molar fractions
Nitrogen	0	0	0.04
Methane	0	0	0.875
Ethane	0	0	0.055
Propane	0	0	0.021
n-Butane	0	0	0.005
Isobutane	0	0	0.003
Isopentane	0	0	0.001
Water	1	1	0
Mass flowrate (t/h)	189	26	3.96
Temperature (°C)	15	15	40
Pressure (bar)	1.5	1.5	70

✓ Compressors

	K101	K 102
Supplied specification	Pressure	Pressure
Exhaust pressure (bar)	10	24.4
Isentropic efficiency	0.805	0.8
Mechanical efficiency	0.97	0.97
Electrical efficiency	0.99	0.99

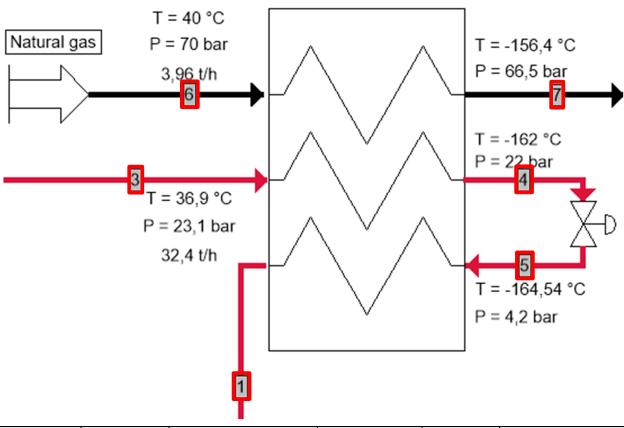
✓ Generalized heat exchangers

	INTERC 101	COND 101
Exchanger type	Counter current or multipasses	Counter current or multipasses
Specification type	Outlet molar vapor fraction on hot stream	Outlet temperature on hot stream
Specification	1	36.9 °C

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✓ MHX "E 100"



Index	Inlet stream	Outlet stream	Туре	Temperature (°C)	Pressure drop (bar)	Pressure profile
	6	7	Outlet temperature	-156.4	3.5	Constant Delta P/
1	U	,	Outlet temperature	-130.4	3.3	Delta H
	3	4	Outlet temperature	-162	1.1	Constant Delta P/
2	3	4	Outlet temperature	-102	1.1	Delta H
	5	1	Outlet temperature	33.9	0.2	Constant Delta P/
3	o	l	Outlet temperature	33.9	0.2	Delta H

✓ Expansion valves

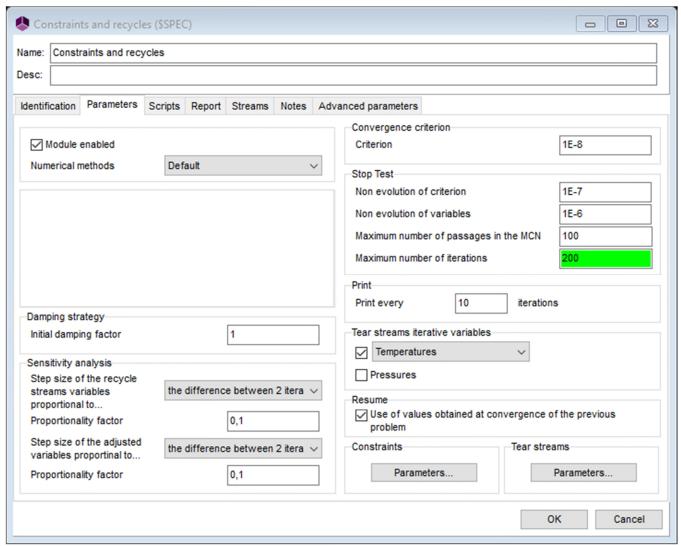
	VLV 101	VLV 201
Constraint type	Pressure specification	Pressure specification
Supplied pressure specification (bar)	4.2	1.2

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✓ Liquid-vapor separator "V 201"

Flash type	Constant pressure and enthalpy flash	
Heat duty specification	Adiabatic	
Pressure specification	The lowest of the feed streams	

✓ Management of constraints and recycles ("SPEC"). The feed flowrates of the cold utility for "COND101" and "INTERC 101" heat exchangers are adjusted in order to reach a temperature of 25°C for the utilities outlets. Therefore, the "Measurement" modules are placed on these two outlets streams and return the deviation between this set point and the simulated value. The "SPEC" modules automatically adjust the flowrates of the feeds modules to satisfy these constraints. The configuration of these "SPEC" modules are the following:



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✓ Energy pinch analysis "Energy pinch analysis"

Pinch (ΔT_{min}) (°C)	10
---------------------------------	----

The process outlet streams and the cold utility streams entering into the two cooling heat exchangers ("INTERC 101" and "COND 101") are not included in the pinch analysis:

Stream name	From	То
9	V 201	LNG
10	V 201	Purge
11	CW Inlet	COND 101
12a	COND 101	Measurement
12b	Measurement	CW outlet
13	CW inlet 2	INTERC 101
14a	INTERC 101	Measurement 1
14b	Measurement 1	CW outlet 2

[✓] Exergy balance "Exergy balance"

All equipment are taken into account for the exergy analysis of the process. Default settings are used to configure the module.

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1.6. Initialization

The calculation sequence is automatically determined by ProSimPlus. Two tear streams are detected: stream "1" (outlet of MHX "E100" and inlet of compressor "K 101") and stream "4" (outlet of MHX "E100" and inlet of valve "VLV 101"). These streams being the streams of the refrigeration cycle, it is necessary to inform their characteristics in terms of compositions and flow rates. The following values are used:

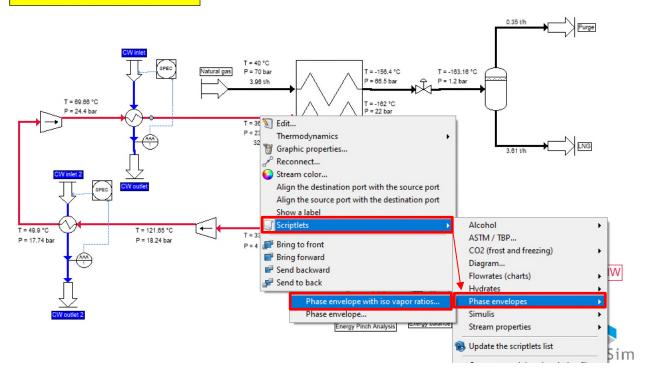
Stream	1	4				
Molar fractions	Molar fractions					
Nitrogen	0.117	0.117				
Methane	0.284	0.284				
Ethane	0.307	0.307				
Propane	0.14	0.14				
n-Butane	0.057	0.057				
Isobutane	0	0				
Isopentane	0.095	0.095				
Water	0	0				
Mass flow rate (t/h)	32.4	32.4				
Temperature (°C)	33.9	-162.0				
Pressure (bar)	4	22				

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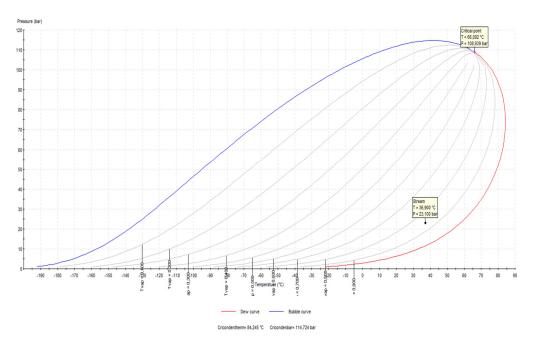
1.7. "Tips and tricks"

The "Phase envelopes" scriptlet allows to draw the phase envelope of a selected stream:

Natural gas liquefaction PRICO process







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2. RESULTS

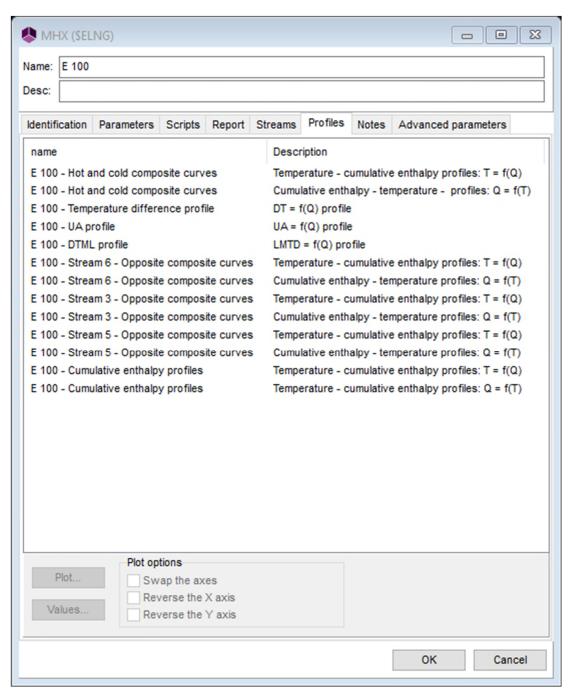
2.1. Process performance

Gas input (t/h)	3.96
Liquefied gas output (t/h)	3.61
Gas recovery ratio (%)	91
Liquefied gas outlet temperature (°C)	-163.16

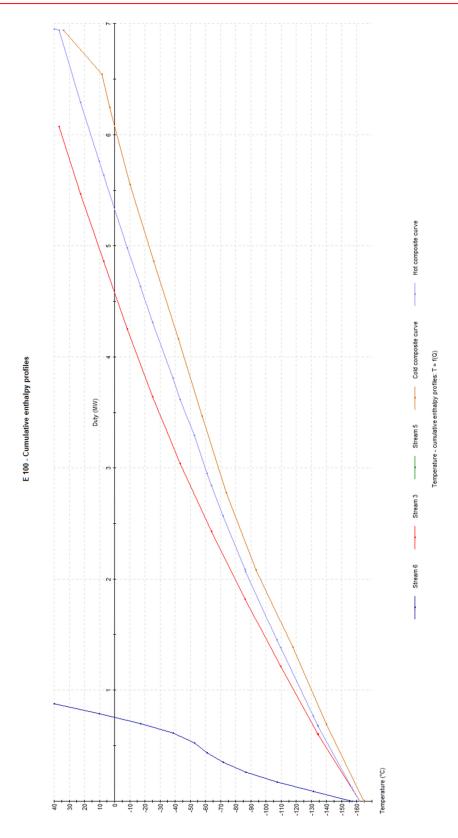
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2.2. Multi-fluid heat exchanger

The profiles of the multi-fluid heat exchanger are accessible after the simulation convergence in the configuration window of the "MHX" equipment, under the "Profiles" tab. Double-clicking on the desired profile generates the graph:



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The cold and hot composite curves are built from the curves of the hot and cold streams. The principle of construction of composite curves and the calculation of the multi-fluid heat exchanger are based on the pinch analysis (see 2.3).

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2.3. Pinch method

2.3.1. Reminders

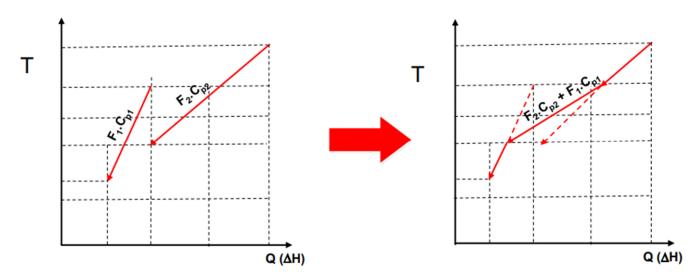
Pinch analysis or Pinch technology is a rigorous and structured method for optimizing the energy expenditure of a process.

The main characteristic of Pinch analysis is to determine, for a particular process or for the whole plant, the minimum consumption of energy, water and hydrogen necessary for its operation. It is therefore possible to assess the maximum potential for improvement, even before starting detailed design work. The method can be applied systematically for each process of the plant or globally for the entire site.

Typical savings identified with a Pinch analysis in industrial sectors such as petroleum refining, chemicals, steel, pulp and paper, petrochemicals, and agribusiness are in the range of 10-35% [CAN03].

The first step of the pinch method is to construct the composite curves. To draw these curves, it is necessary to know the values of the flow rates of the streams F, their specific heat capacity \mathcal{C}_p , and the inlet and outlet temperatures (ΔT) for each heating and cooling of the process. The composite curves represent the profile of the available heat sources ("hot composite curve") and the profile of the thermal requirements of the process ("cold composite curve"). Depending on their shape and location, these curves provide information on the possibilities for heat recovery within the process.

The following figure shows the construction of the hot composite curve on a Temperature-Quantity of heat exchanged diagram. The hot composite curve is constructed simply by adding, for each temperature interval, the changes in thermal load of each of the streams taken individually.



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The construction is based on the following equation:

$$Q = FC_{v}\Delta T$$

With:

Q : Quantity of heat duty exchanged (W)

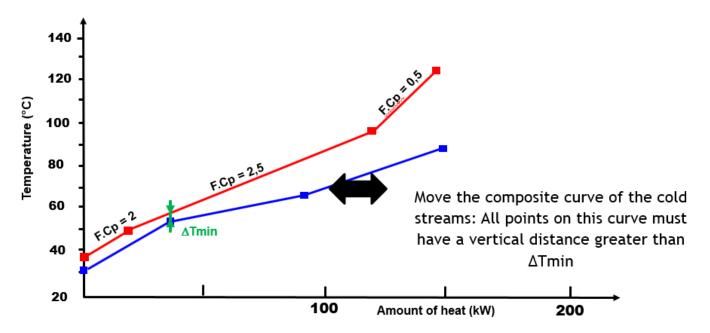
F: Flow rate of the heated stream or the cooled stream (kg/s)

 C_p : Specific heat of the stream (J/kg/°C)

 ΔT : Temperature difference between the inlet and the outlet of the heating or cooling (°C)

The cold composite curve is obtained in the same way.

To establish the minimum energy consumption target for the process under study, the cold composite curve is positioned on the same diagram as that of the hot composite curve.

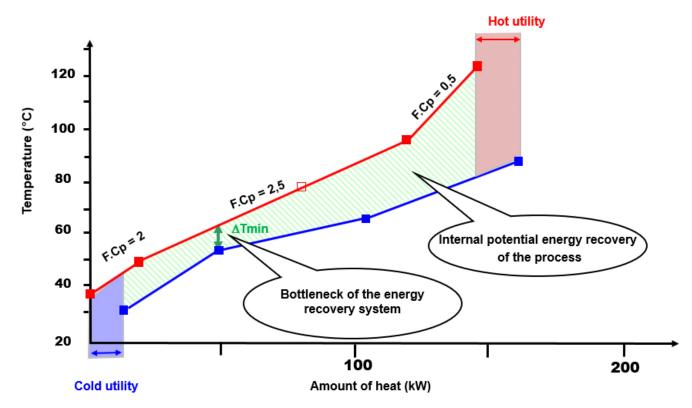


The 2 curves are slided horizontally until there is a certain difference between the 2 curves. The hot composite curve must be above the cold composite curve (for heat exchange to be possible). The smallest difference between the two curves (the locus where they are close) is the temperature difference Δ Tmin also called the pinch. This value indicates the minimum temperature difference that is acceptable between the two fluids in a heat exchanger. This pinch value varies depending on the processes and heat exchanger technologies used in each process (from 10 to 20°C for petrochemicals, from 3 to 5°C for cryogenics...).

The overlap area of the two curves represents the Maximum of Energy Recovery (MER). The areas outside the overlap area represent the amounts of energy requirement to be supplied by the utilities.

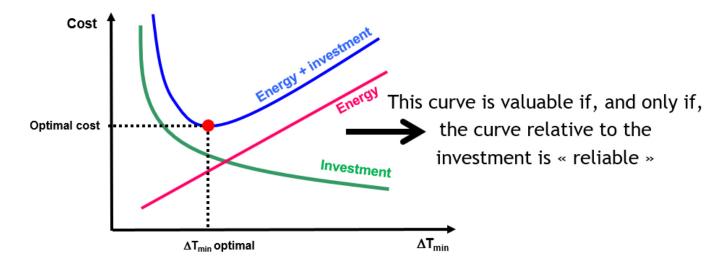
Pinch analysis therefore makes it possible to establish targets for the minimum energy consumption necessary to meet the needs of a process, even before starting the design of the heat exchanger network. This allows to quickly identify the extent of energy savings that can be considered at an early stage of the analysis. This advantage is probably the most interesting that Pinch analysis offers.

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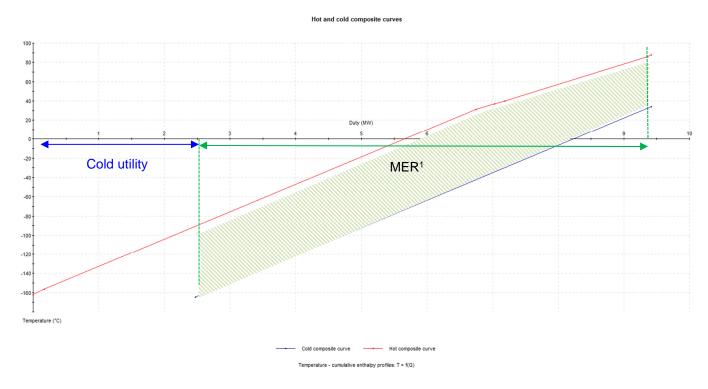
As the two composite curves move apart, the pinch increases, and therefore the temperature differences between hot streams and cold streams increase. It then becomes possible to reduce the exchange surfaces of the heat exchangers for the recovery of MER and therefore to reduce the cost of heat exchangers (investment). Conversely, the greater the pinch is, the lower the MER (overlap zone) is. The process then consumes more hot and cold utilities and the energy cost increases when pinch increases too.

The following figure shows that there is an optimal value for the pinch, which minimizes the total cost, taking into account the expenses related to the investment and those related to energy [CAN03].



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2.3.2. Results



¹ MER: Maximum of Energy Recovery

The hot and cold composite curves plotted above are used to identify the relevant energy recoveries using the pinch method (see 2.3.1). The overlap zone between the two curves (green zone) indicates the quantity of energy that it will be possible to save with internal energy recoveries by associating in the most judicious way the "energy sources streams" (hot streams) with "energy sinks streams" (cold streams). On the left of the diagram, the deviation between the two curves shows the minimum cold utility requirement necessary for the process if 100% of the MER is recovered by an efficient network of heat exchangers. It is also possible to notice the absence of hot utility for this process (cf. 2.3.1).

Heat duty of the « MHX » module (MW)	6.95
Heat duty of the « INTERC 101 » exchanger (MW)	0.93
Heat duty of the « COND 101 » exchanger (MW)	1.53
Global amount of energy extracted by cold utilities (MW)	2.46

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By comparing the values of the composite curves and the quantities of energy exchanged in each module, it is possible to notice that the entire amount of recoverable energy (Maximum of Energy Recovery) is recovered by the MHX multi-fluid heat exchanger. The minimum cold utility requirement corresponds to the quantities of heat duty exchanged in the two cooling exchangers.

By checking the box "Integration potential printing" in the advanced options of the module, it is possible to know the amount of energy supplied and extracted by the cold and hot utilities for the simulated process. For this process, 2.47 MW are currently extracted by cold utilities, 100% of the energy that could be saved theoretically is really, since it is equal to the minimum utility quantity.

		HEAT DUTY (MW)		CATTERACTION DATES (%)	
	MINIMUM	ACTUAL	MAXIMUM	SATISFACTION RATIO (%)	
COLD FLUID	2.47416	2.47416	9.41577	73.723	
HOT FLUID	0.00000	0.00000	6.94161	100.000	

Maximum energy recovery	=	6.94161	(MW)
Pinch temperature	=	59.2641	(°C)
Real integration ratio	=	100.000	(%)
Integration potential indicator #1	=	84.874	(%)
Integration potential indicator #2	=	73.723	(%)

Note: The pinch of 10°C specified by the user is not reachable for this simulation. Indeed, the translation of the cold composite curve below the hot composite curve to reach a pinch of 10°C would create 2 levels of cold utilities on both sides of the MER. In consequence, the translation of the cold composite curve under the hot composite curve is possible until the demand for hot utility is zero (with only one cold utility requirement placed on the left side of the hot and cold composite curves graph).

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2.4. Exergy analysis

2.4.1. Reminders

The exergy is the theoretical maximum of recoverable work when a system is brought, from its initial state to the state of thermodynamic equilibrium in a reference environment (at a temperature T^{00} of 25°C and a pressure P^{00} of 1 atm). More intuitively, exergy represents the quality of a type of energy. For example, 1 kWh of electricity is not equivalent to 1 kWh of heat and 1 kWh of heat at 100°C is not equivalent to 1 kWh of heat at 40°C because the potential for use and recovery are not the same.

The exergy of a material flow is noted B (J/mol) and is expressed as:

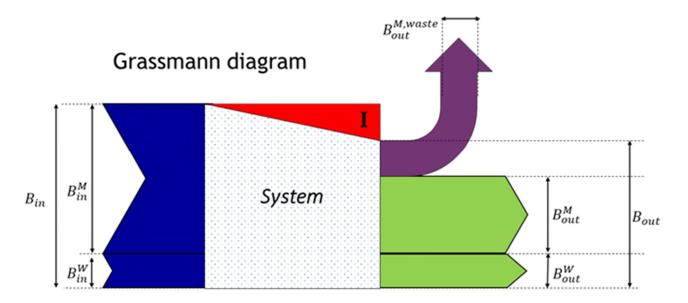
$$B = H - T^{00}S$$

With:

H: Enthalpy (J/mol)

S : Entropy (J/mol/°C)

According to the 1st principle of thermodynamics, the energy of a closed system is conserved during a transformation and the entropy of a system only increases during thermodynamic transformations according to the 2nd principle of thermodynamics. Unlike an energy balance, the exergy balance is therefore not conservative. The exergy entering in a system is equal to the sum of the exergy exiting and the irreversibility created. The exergy only decreases during real thermodynamic transformations. The exergy balance is generally represented using a Grassmann diagram:

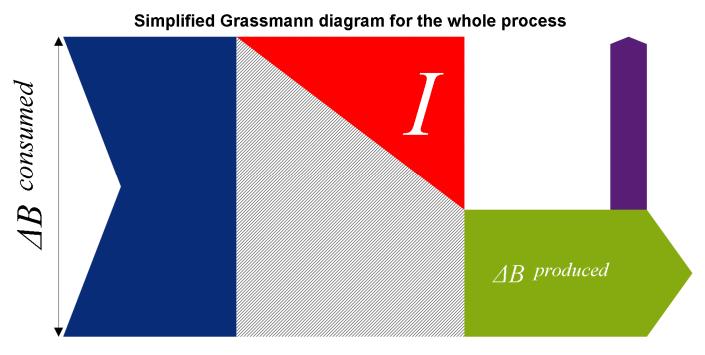


The exergy can therefore only decrease during a real non-reversible transformation. The lost exergy represents the irreversibility of the process: the less irreversibility created, the greater the exergy and efficiency and the closer the process is to "ideality". The exergy analysis therefore makes it possible to carry out an energy diagnosis of the process by mapping the thermodynamic irreversibilities of a system [GOU15].

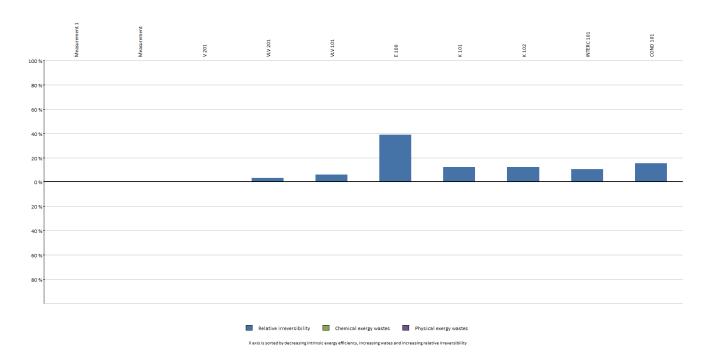
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2.4.2. Results

The exergy balance of this process is displayed using a "Grassmann" diagram:

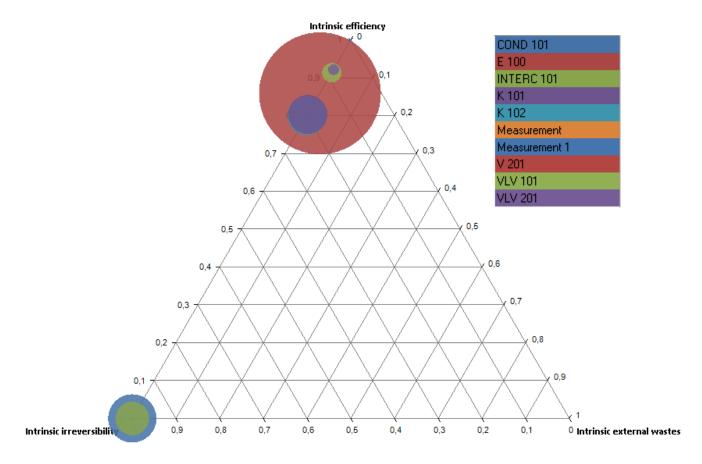


The following graph is used to detect the irreversibilities of each unit operation of the process:



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The following graph is used to display the performance and efficiency coefficients of each unit operation of the process:

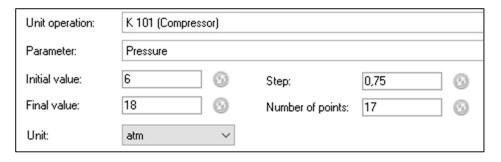


It should be noted that the graphs presented in this paragraph are part of the results generated automatically by the exergy balance module (accessible in the "Balance results" tab of the module).

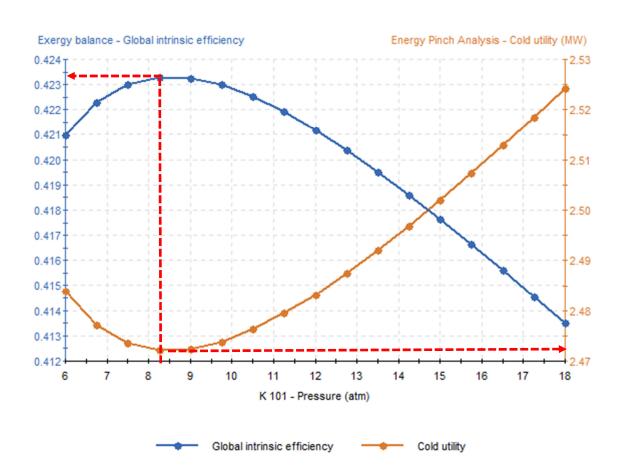
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2.5. <u>Case studies</u>

A case study was performed to observe the impact of the pressure modification on the outlet of the first refrigerant compression stage (K101). The parameters monitored are the exergy efficiency of the exergy analysis module and the amount of cold utilities of the pinch analysis module. For these two monitored parameters, a pressure of 8.25 atm seems optimal for the K 101 compressor. This value minimizes the amount of cold utility required, and maximizes the exergy efficiency of the process. The case study is configured as below and the results "Overall intrinsic efficiency" (of the exergy balance module) and "Quantity of cold utilities" (of the energy pinch analysis module) are monitored:



Exergy balance - Global intrinsic efficiency Energy Pinch Analysis - Cold utility (MW)



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